

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 10.6

Global applicability domain: Inside

Local applicability domain index: 9.79e-01

Confidence level: 5.70e-01

Nearest Neighbors from the Training Set

Image not found

2,2'4,4'-Tetrabromodiphenyl ether

Measured: 10.5
Predicted: 10.6

Image not found

1,2,3,4,5,6,7,8-Octachloronaphthalene

Measured: 11.1
Predicted: 10.6

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1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin

Measured: 11.0
Predicted: 10.2

Image not found

1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin

Measured: 11.0
Predicted: 10.2